Numerical Simulation of Biomass Gasification in a Steam-Blown Bubbling Fluidized Bed

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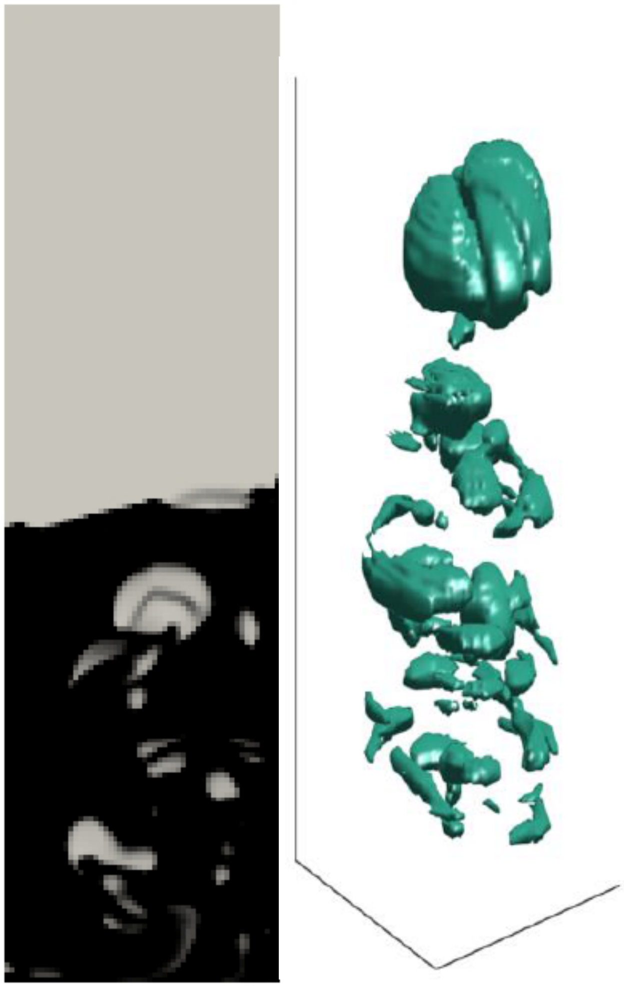
Steam-blown fluidized bed gasifiers



Fluidized bed: Favorable reactor technology for biomass gasification with minimum pretreatment

Advantages:

- High levels of intermixing
- Suitable for coarse particles with large residence times

Disadvantages:

- Lower levels of carbon conversion with considerable tar content

Steam as a gasification agent:

Advantages:

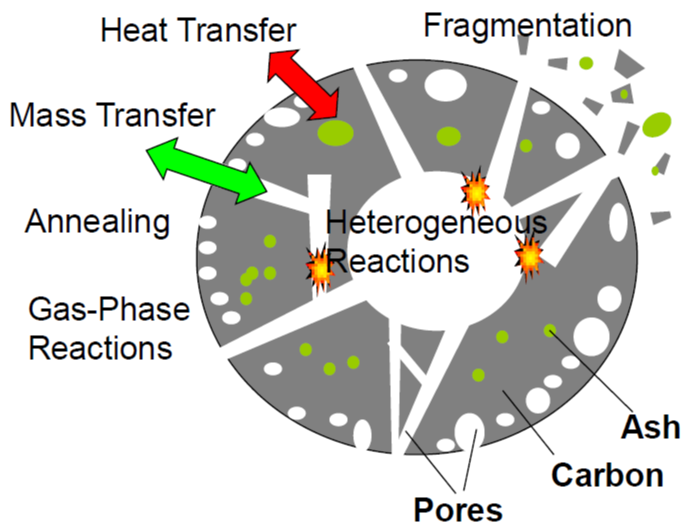
- Reduced cost, no air separation is needed
- In the absence of oxidation, hot zones are avoided in the bed

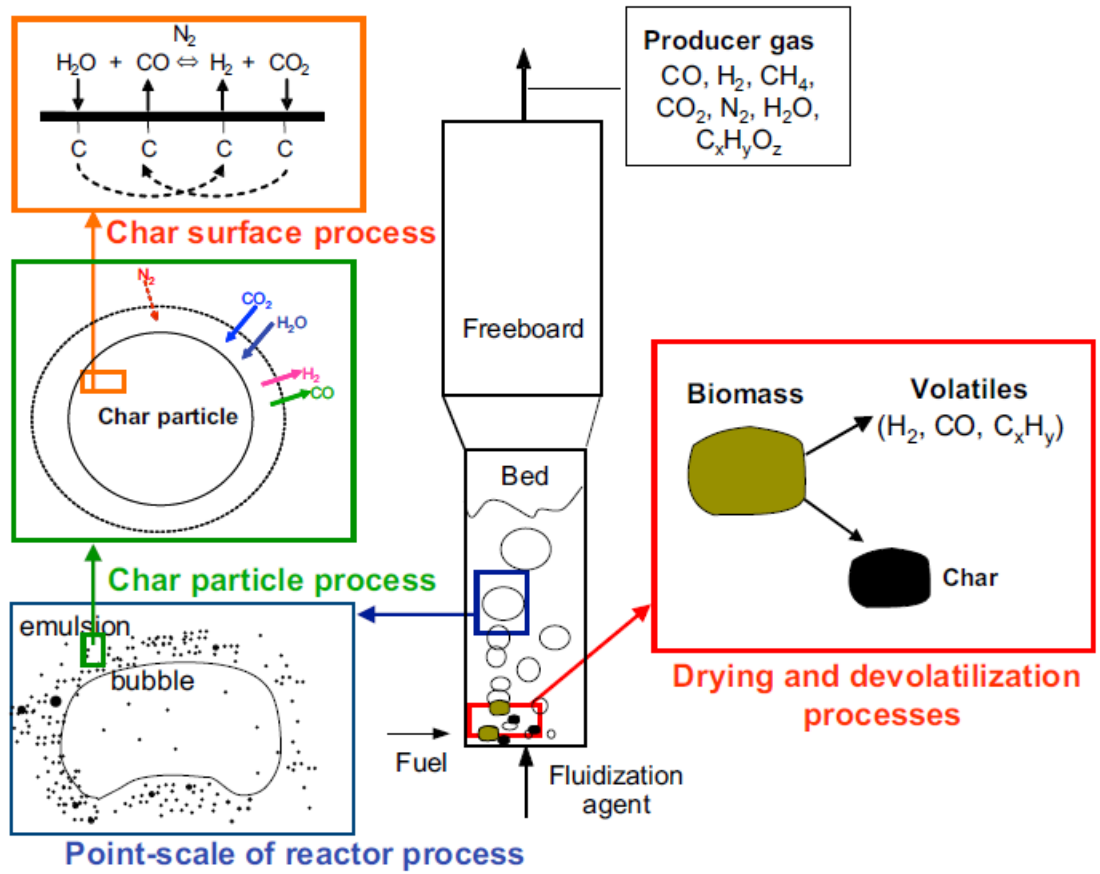
Disadvantages:

- Biomass devolatilization and char gasification are endothermic
- External heating is needed for controlling the process

Key phenomena in a fluidized bed gasifier

Multi-scale process:
- Gas-phase chemistry
- Surface chemistry
- Single-particle modeling
- Hydrodynamics



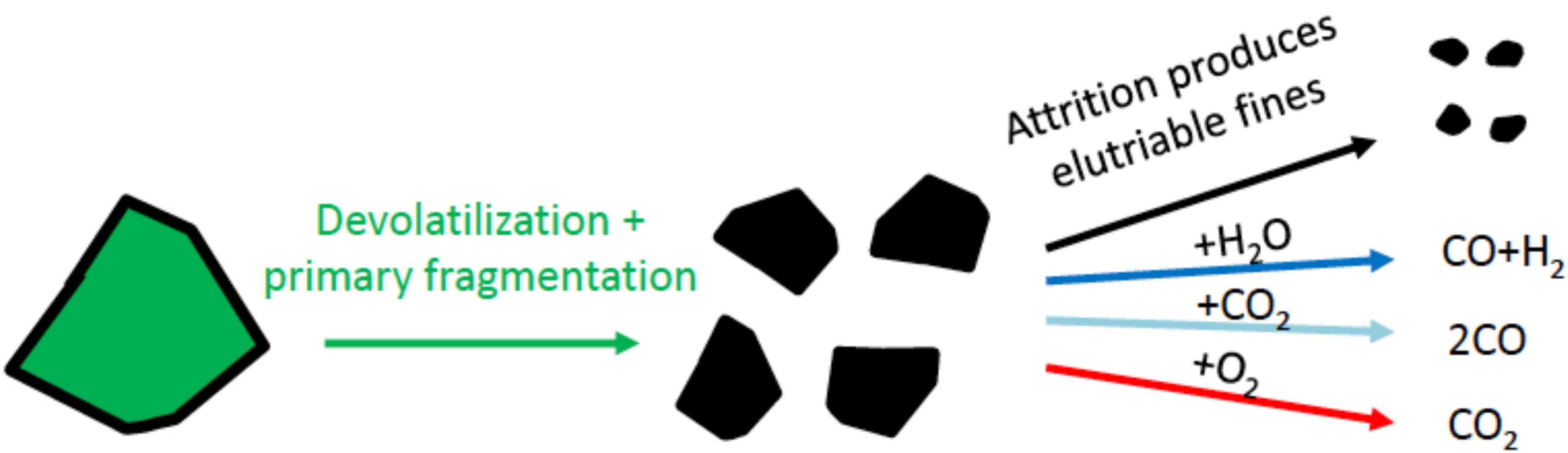


Goal

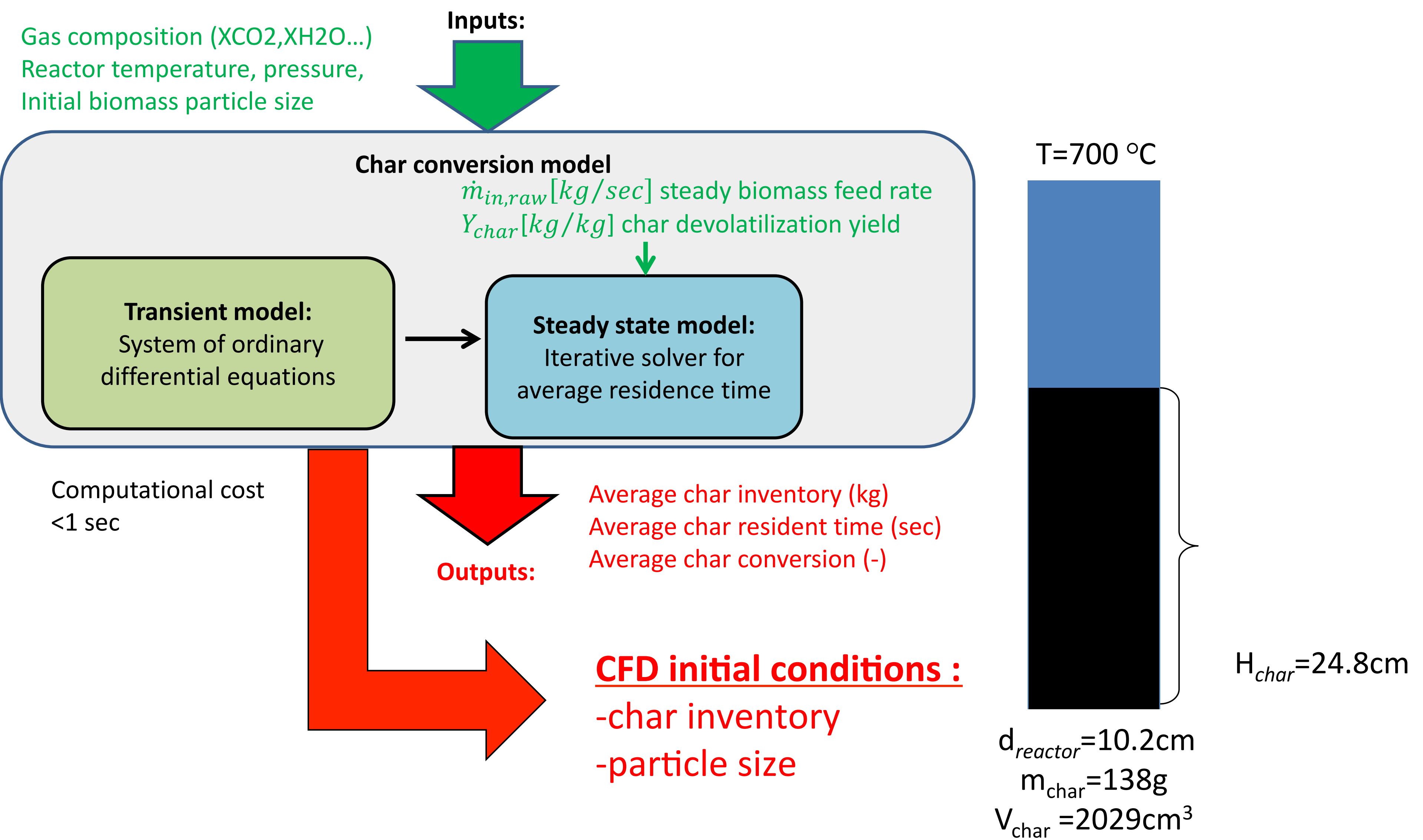
- Development of a multiscale CFD methodology for the reactive multiphase simulations to assist the design and optimization of gasification processes by reducing the cost, compared with experiments, and offering information for integration in ROM

Modeling Challenges: Initial char loading

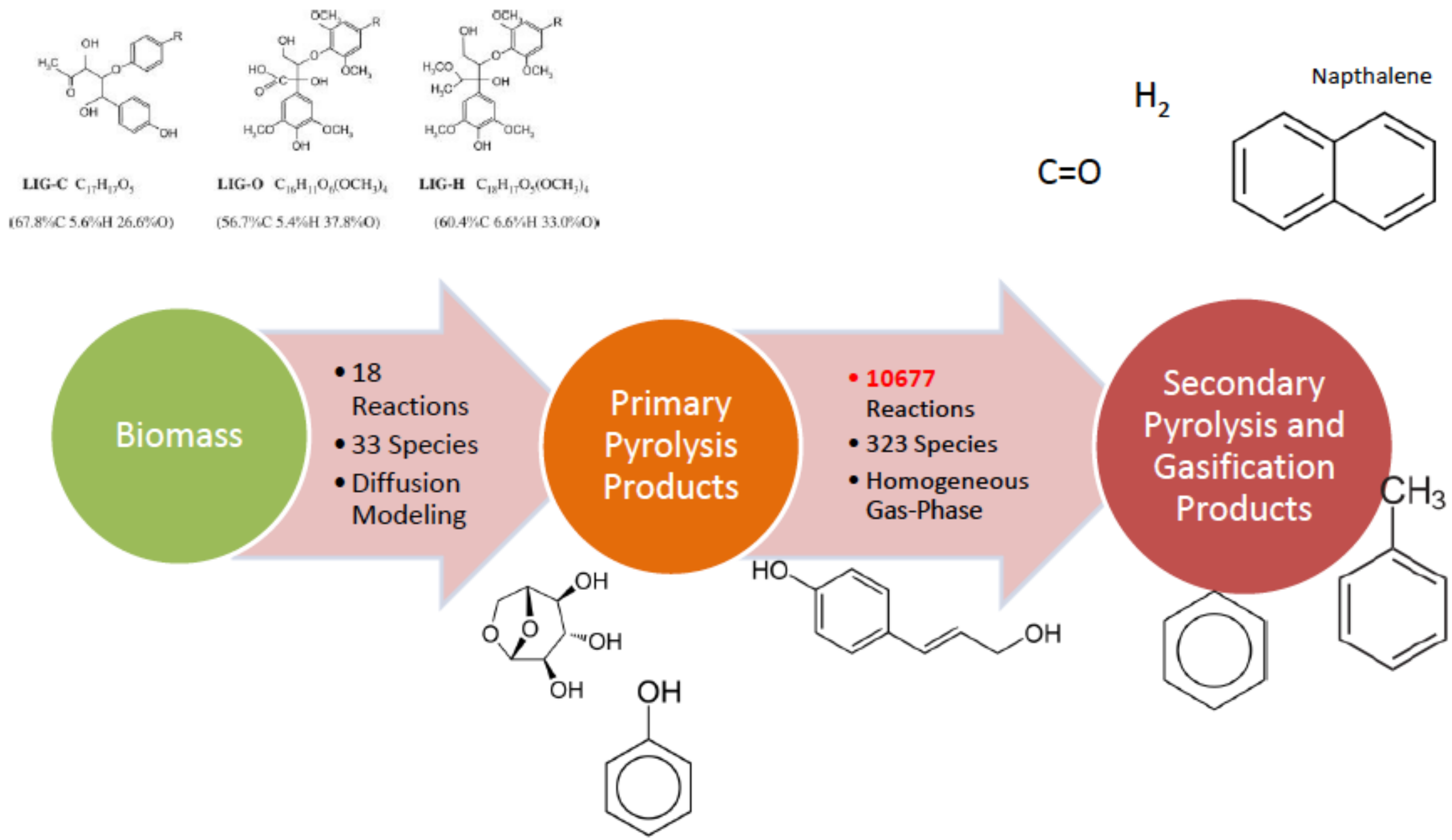
- **Challenge**: Steady state char inventory takes hours to reach for gasification conditions
  - Initial transient too long for CFD simulation
- **Solution:** Standalone MATLAB steady state char conversion model computes char inventory for CFD initial condition
  - Char gasification and combustion
  - Gasification assisted attrition due to hardness reduction



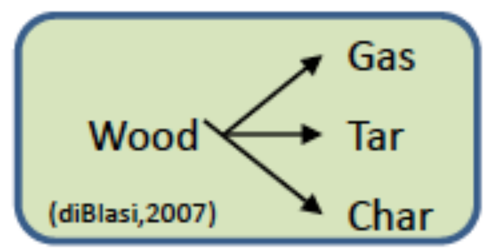
Steady state char inventory for steam blown gasifier



Modeling Challenges: Chemistry description



- Challenge: Number of species/reactions prohibitively large for use in CFD
- Solution: Use of Global models for pyrolysis and tar cracking [1]



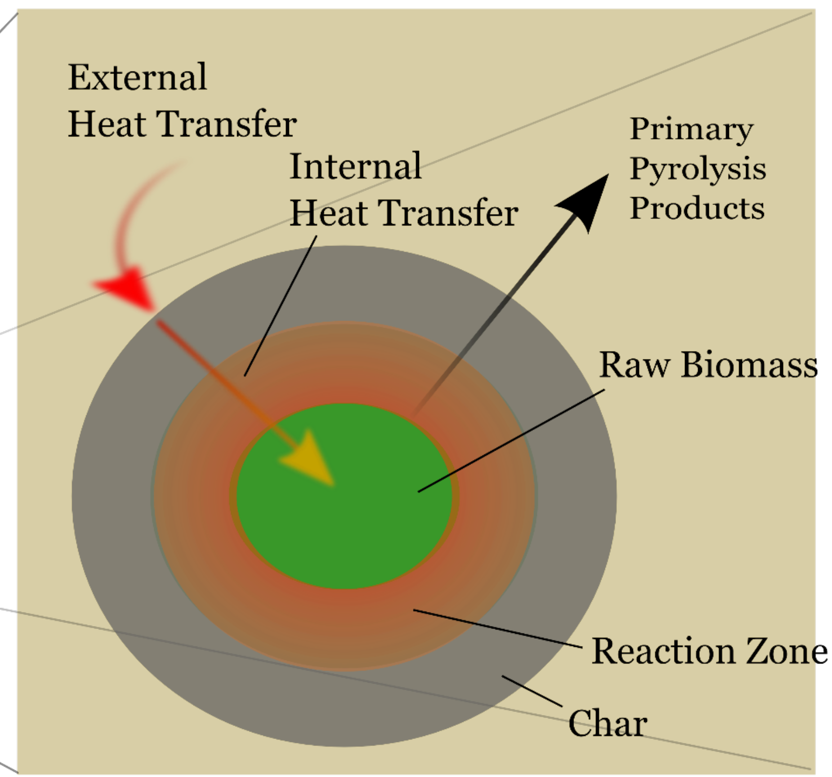
Global devolatilization model

- Devolatilization dynamics are strongly influenced by particle radius.
- Shrinking Core Model Implemented for Eulerian Modeling Framework:

$$k_{eff} = \frac{1}{\frac{1}{k_{kin}} + \frac{a}{k_{cond}}}$$

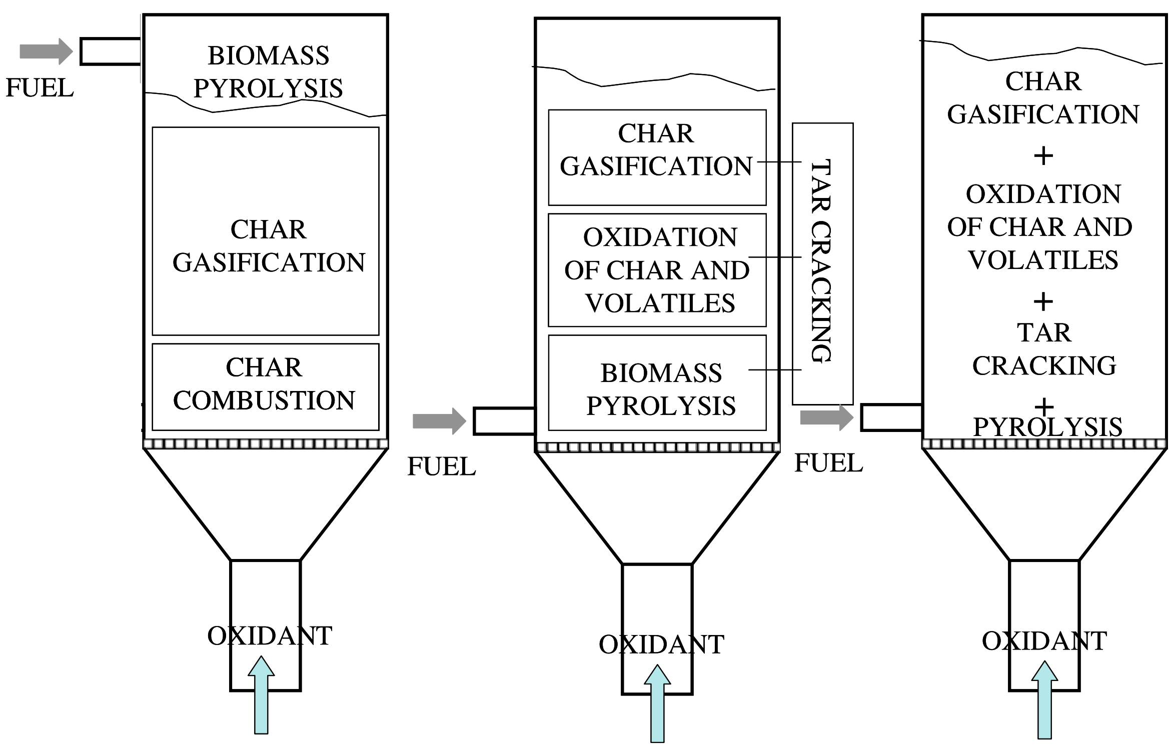
- Trade-off of devolatilization time and mixing time important for well-stirred assumption.

Particle-Scale Devolatilization Modeling Framework



Modeling Challenges: Hydrodynamics

- Raw biomass injected as particles and removed as char
- Biomass typically <2-3% of bed mass
- Bed temperature 600-1000°C
- Very rapid heat up
- **Mixing** and **particle residence times** are very important to product composition and conversion



Devolatilization time scales are similar with mixing time scales, so accurate prediction of the position of raw biomass is important

CFD modeling strategy for gas-particle flows

Two Fluid Model

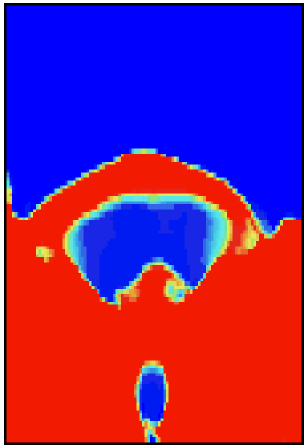
Both phases are considered as fully interpenetrating continua

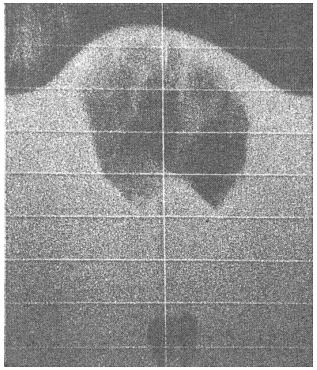
→ Gas Phase → Eulerian Framework
Particle Phase → Eulerian Framework

ADVANTAGE: High computational efficiency makes this method more attractive since parametric and design studies of large-scale systems are feasible

DISADVANTAGE: Closures are required for the modeling of:

- Interphase momentum exchange
- Particle-particle interaction

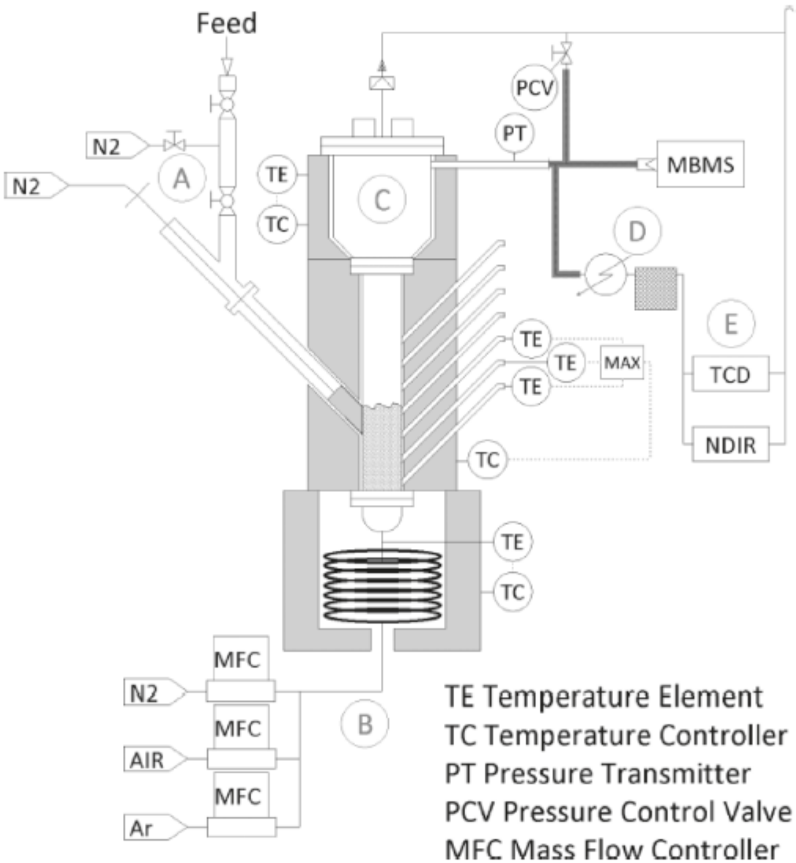




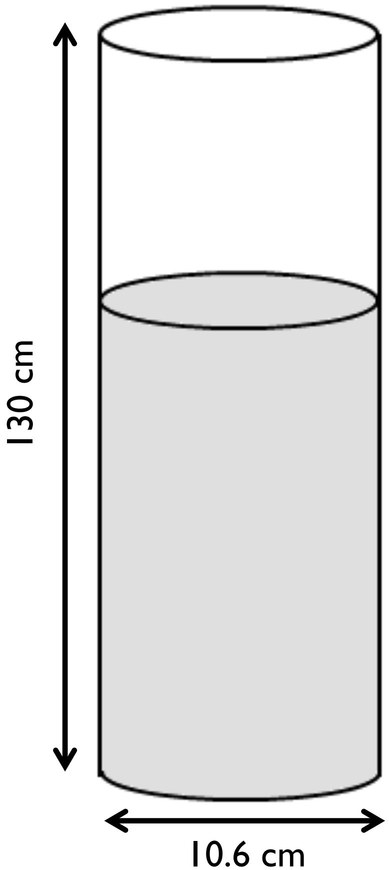
Numerical tool: **MFIX** (DOE-NETL) [2,3]

NREL gasifier

Experimental Parameter	Value
Bed material Size, $d_{p,}$ Density ρ_p	Olivine $(Mg,Fe)_2SiO_4$ 270 µm 3300 kg/m^3
Minimum Fluidization u_{mf}	~0.037m/s
Superficial velocity, $_{,}u_0$	~0.12 m/s
Bed diameter, d_{bed} Bed Height	4''(0.106 m), 0.13m
Bed temperature, T_{bed} (heated walls)	750, 800, 850 °C,
Inlet gas composition X_{feed}	100% H_2O(%vol) <2% Helium
Input biomass feed rate $_{bio,0}$	800g/hour
Biomass mean diameter $d_{bio,0}$	1 mm
Steam flow rate	800g/hour



Simulation setup



- 2D simulations of a steam blown gasifier
(Both reacting and non-reacting)
- 3 solid phases considered
    - Biomass : Rho=600kg/m3, d=1mm
    - Char : Rho=170kg/m3, d=0.38mm
    - Sand : Rho=3300kg/m3, d=0.27mm
- Drag model: Gidaspow
- Inter-particle drag model: Gera et al. 2004 [4]
    - Friction coefficient, C_f = 0.1
    - Segregation slope coefficient, C_s = 0.1
- Partial slip BC for solids
- Specularity coefficient, ϕ = 0.05 [5,6]
- Dirichlet BC for temperature (1023 K) along walls and inflow
- Initial Condition
    - Static bed height: 24.4 cm
    - $\varepsilon_{s,sand}$ = 0.4582
    - $E_{s,char}$ = 0.1218
- Resolution: 40X400 cells

Chemistry description

Chemical mechanism

- Drying

- Devolatilization (Competing pathways following Gronli 2000 [7])

bio --> 7.7872**H_2** + 4.7274**CO** + 4.3016**CO_2** + 1.7109**CH_4** + 6.9712**H_2O**

bio --> 6.2792**tar1**

bio --> 40.8361**FC1**

- Tar cracking (Details in following slides)

- Water gas shift (Fast kinetics Biba 1978 [8])

$CO + H_2O \to H_2 + CO_2$
$H_2 + CO_2 \to CO + H_2O$

- Char gasification (Hobbs 1992 [9])

$C + CO_2 \to 2CO$
$C + H_2O \to CO + H_2$

Tar cracking reaction

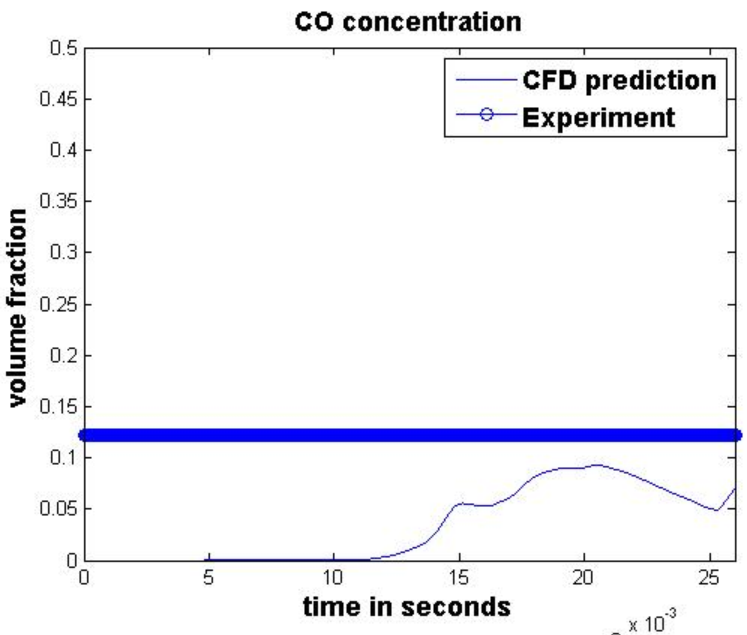
Tar1 → light gases + inert tar

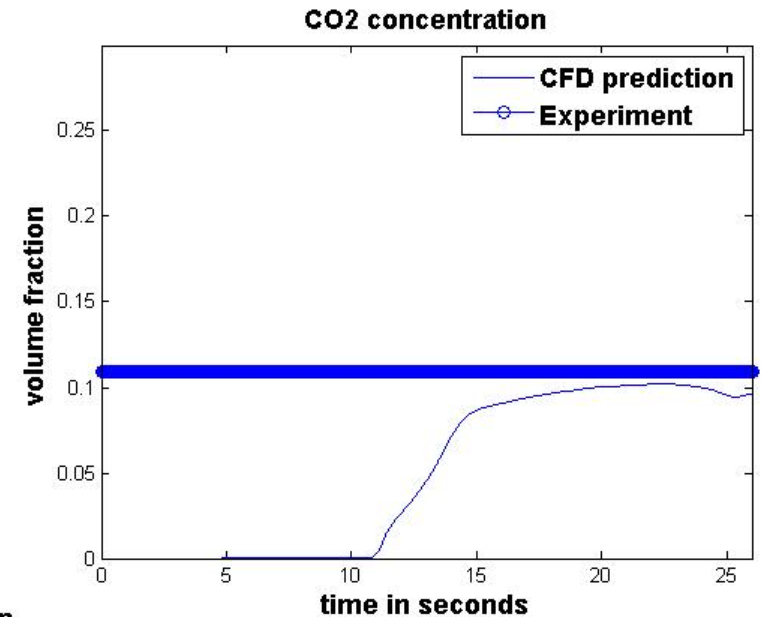
Component mass fraction	Seebauer 1999
Light gases	0.78
Tar_{inert}	0.22

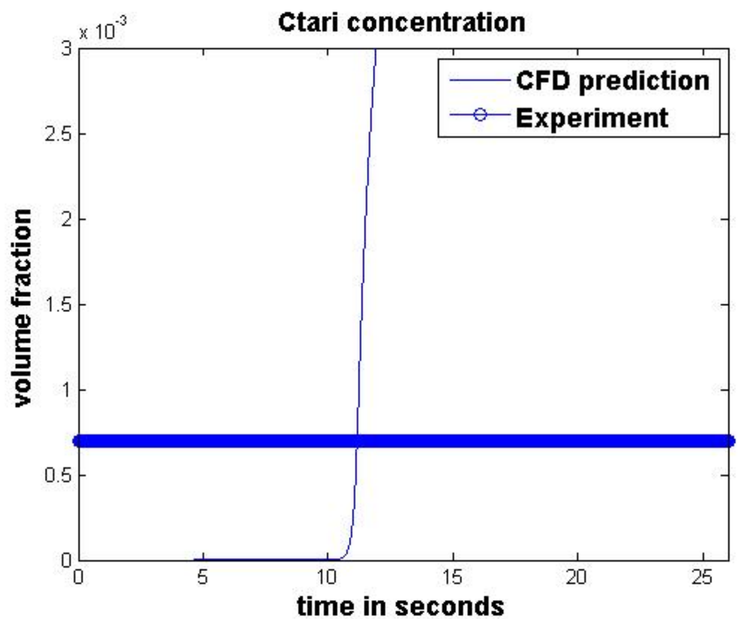
Tar1 → 1.5709**CO**+0.197**CO2** + 0.4304**CH4** + 0.6704**H2**+ 0.22**Tari**

- Both tar1 and tari are considered to be benzene
- The global reaction is developed for biomass pyrolysis in inert environment (N2) at moderate temperatures

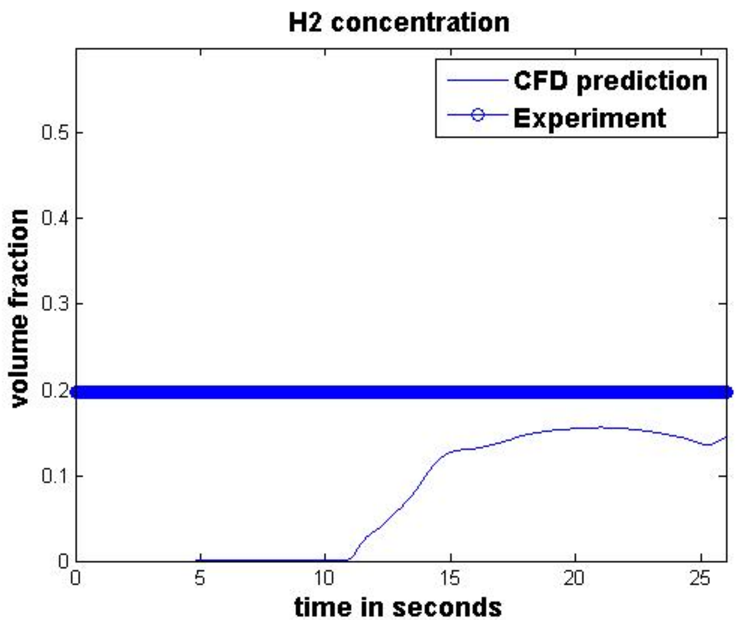
Comparison with NREL experiments, 1023K
Steam blown bed

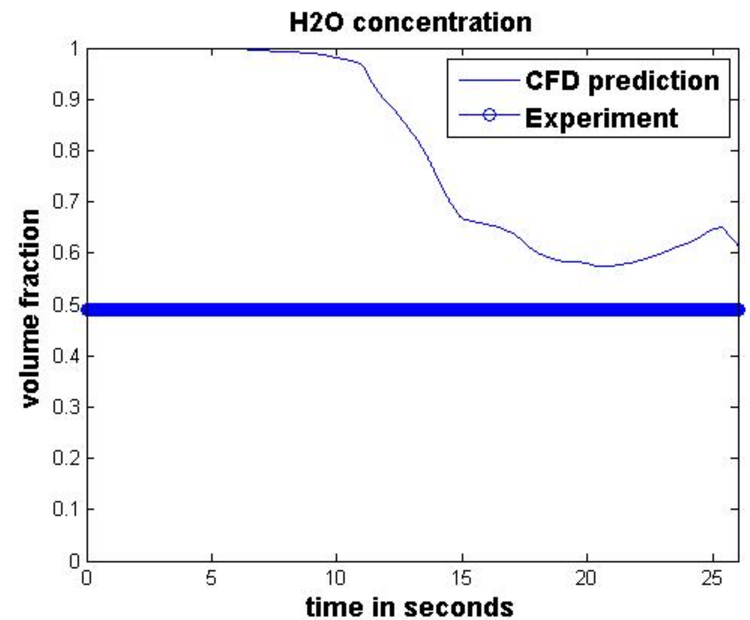






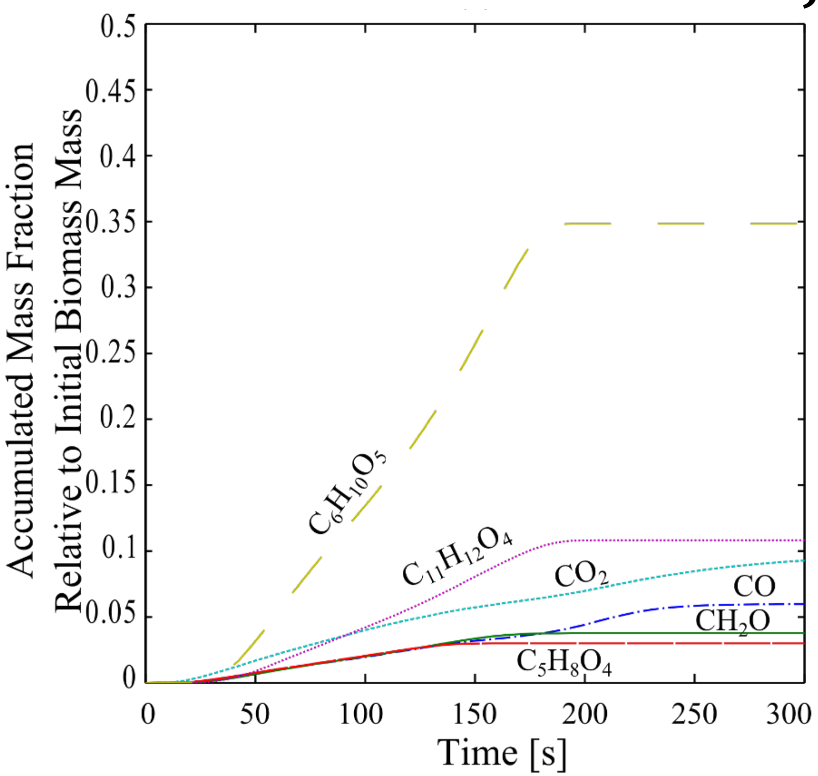
Comparison with NREL experiments, 1023K Steam blown bed

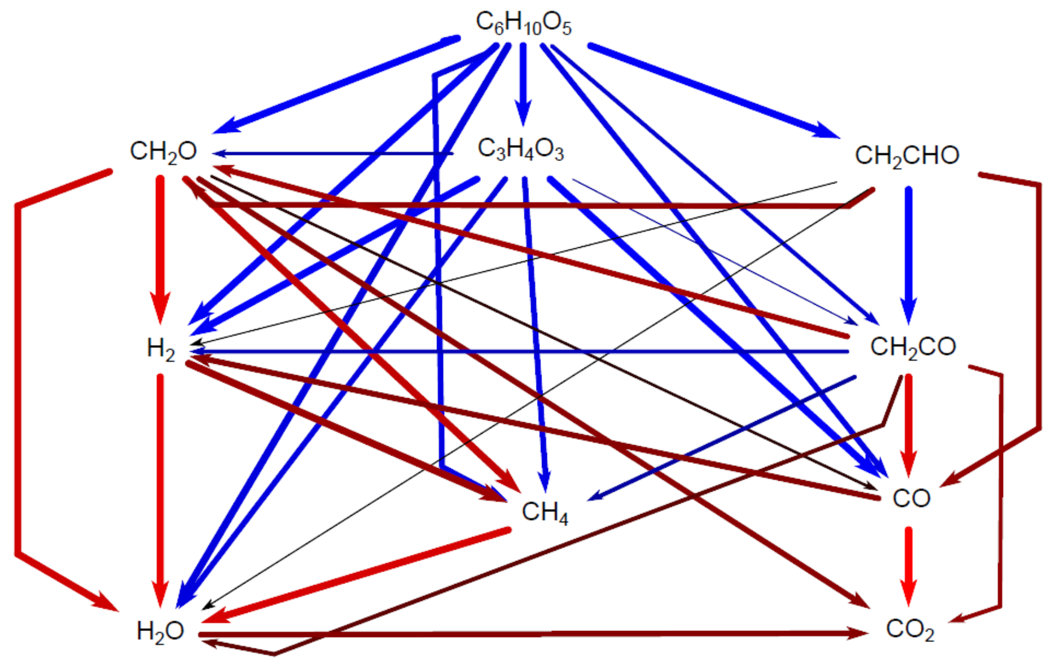




The tar cracking mechanism of Seebauer 1999 over-predicts the produced inert tars by two orders of magnitude

Identification of major tars after devolatilization



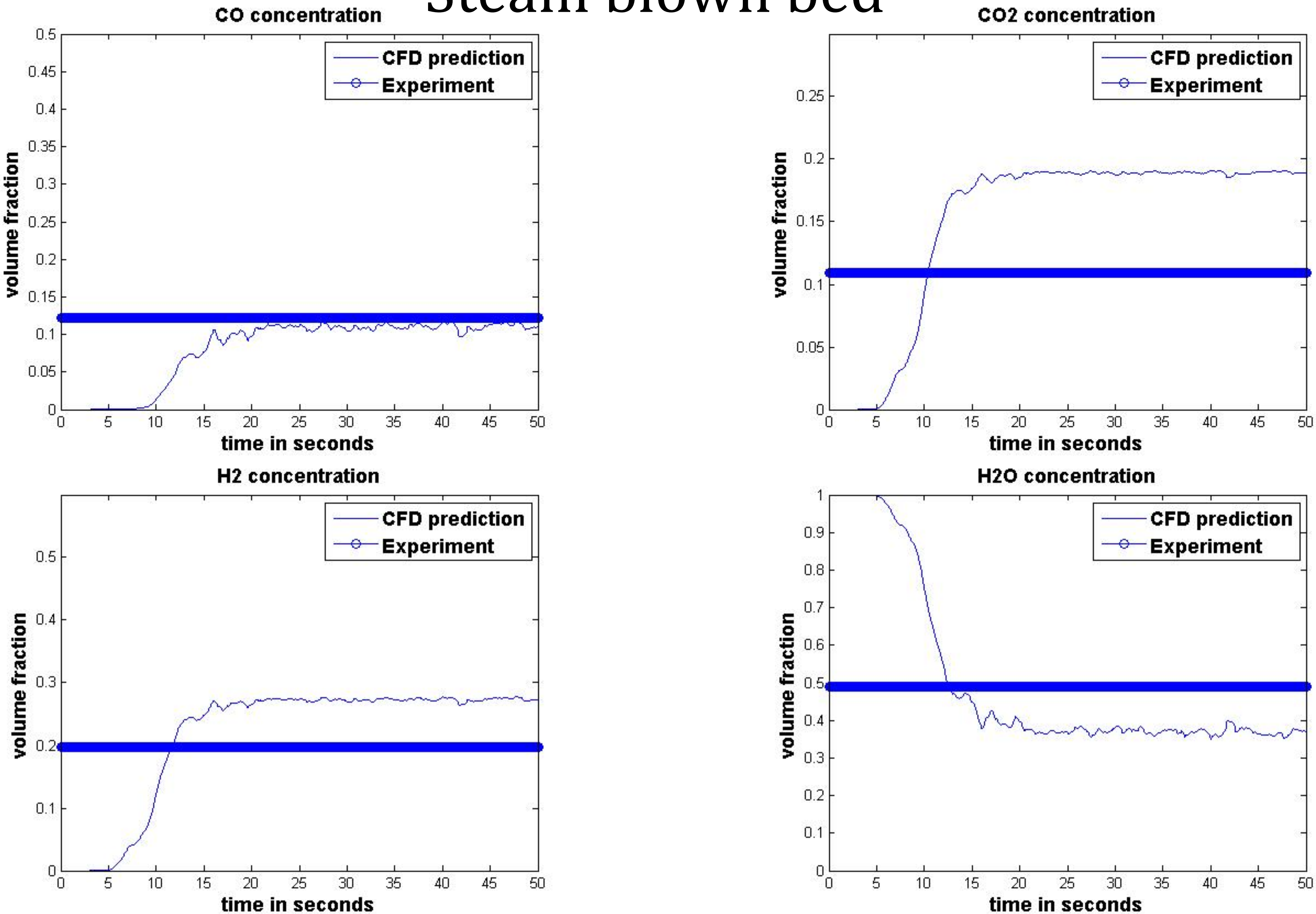


- Levoglucosan identified as a the major tar species present after devolatilization [10]
- Global tar cracking mechanism in a steam environment, based on leveglucosan cracking
- Benzene assumed as the major inert tar species

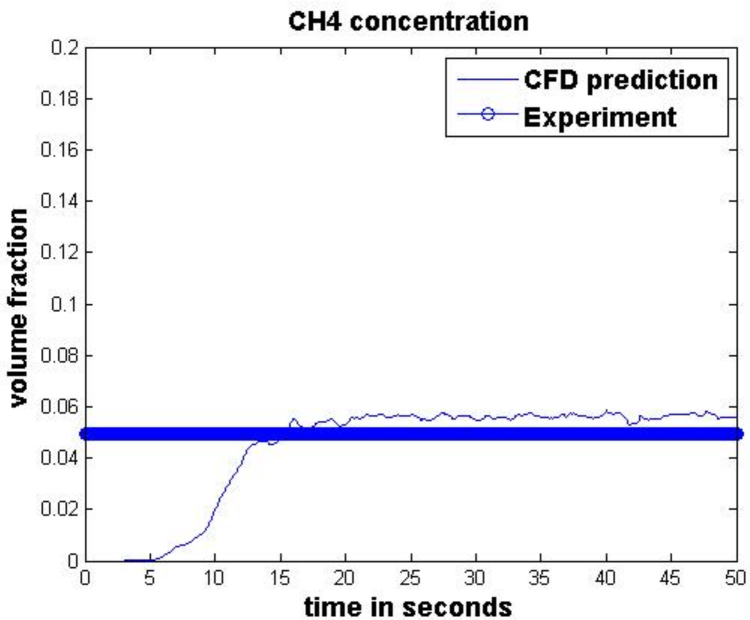
Tar cracking mechanism was modified using a reactor network model employing the Ranzi mechanism to represent the LVG decomposition pattern in the absence of oxygen

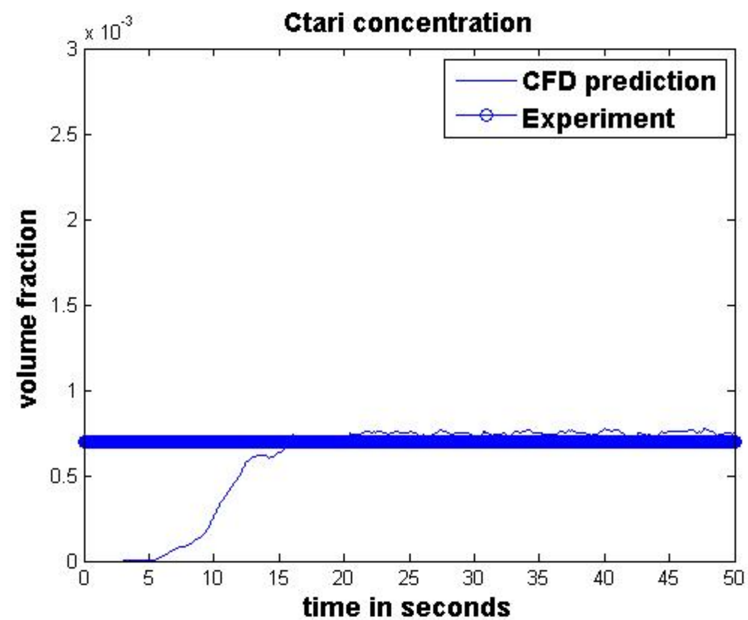
Tar1(LVG) → 3.27**CO** + 0.2**CO2** + 0.65**CH4** + 1.1**H2** + 2.68**H2O** + 0.01038**Tari(Benzene)**

Comparison with NREL experiments, 1023K
Steam blown bed

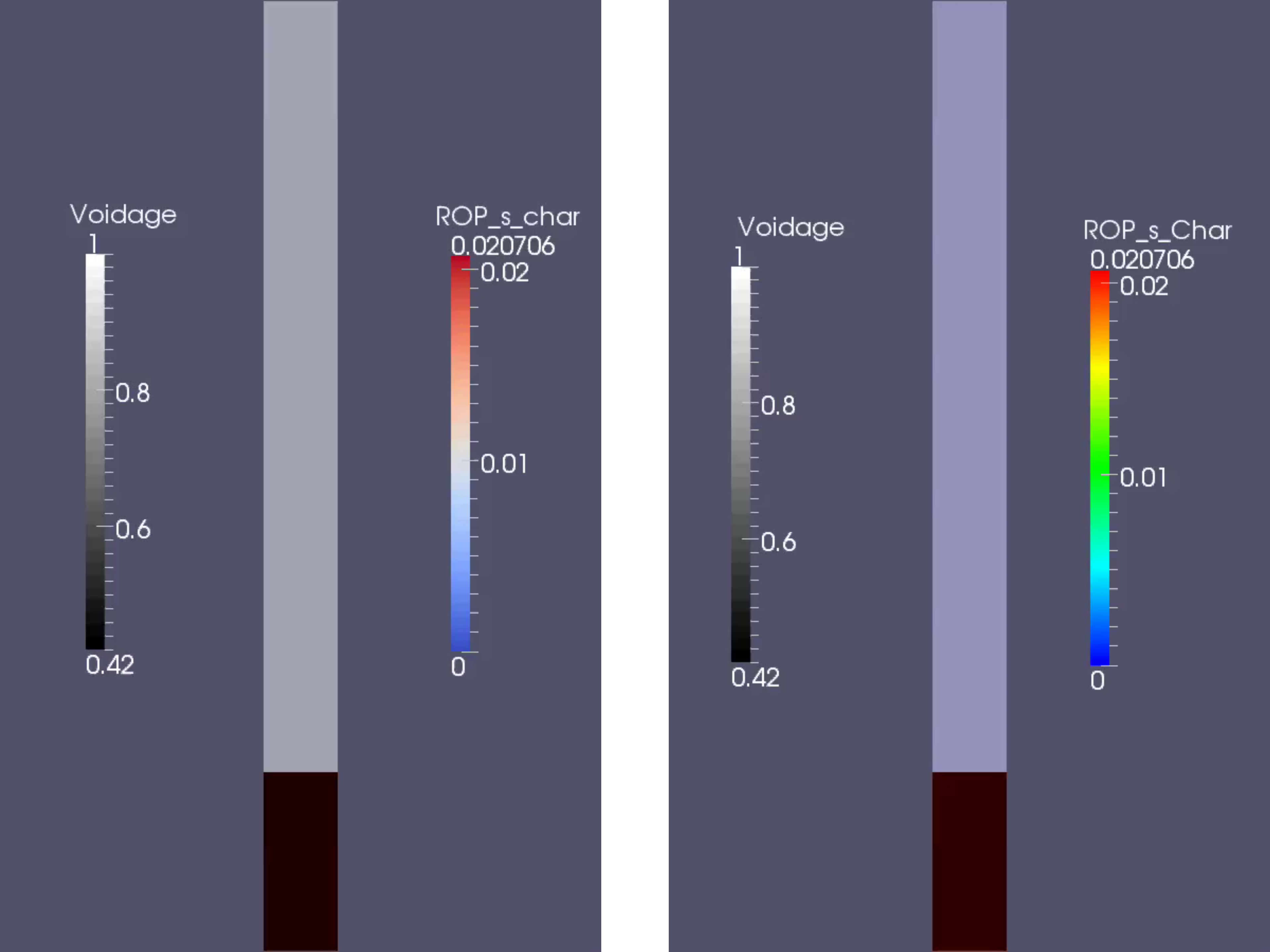


Comparison with NREL experiments, 1023K Steam blown bed





- Tar production is predicted accurately
- Discrepancies for CO_2, H_2 and H_2O


Voidage
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ROP_s_char
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Voidage
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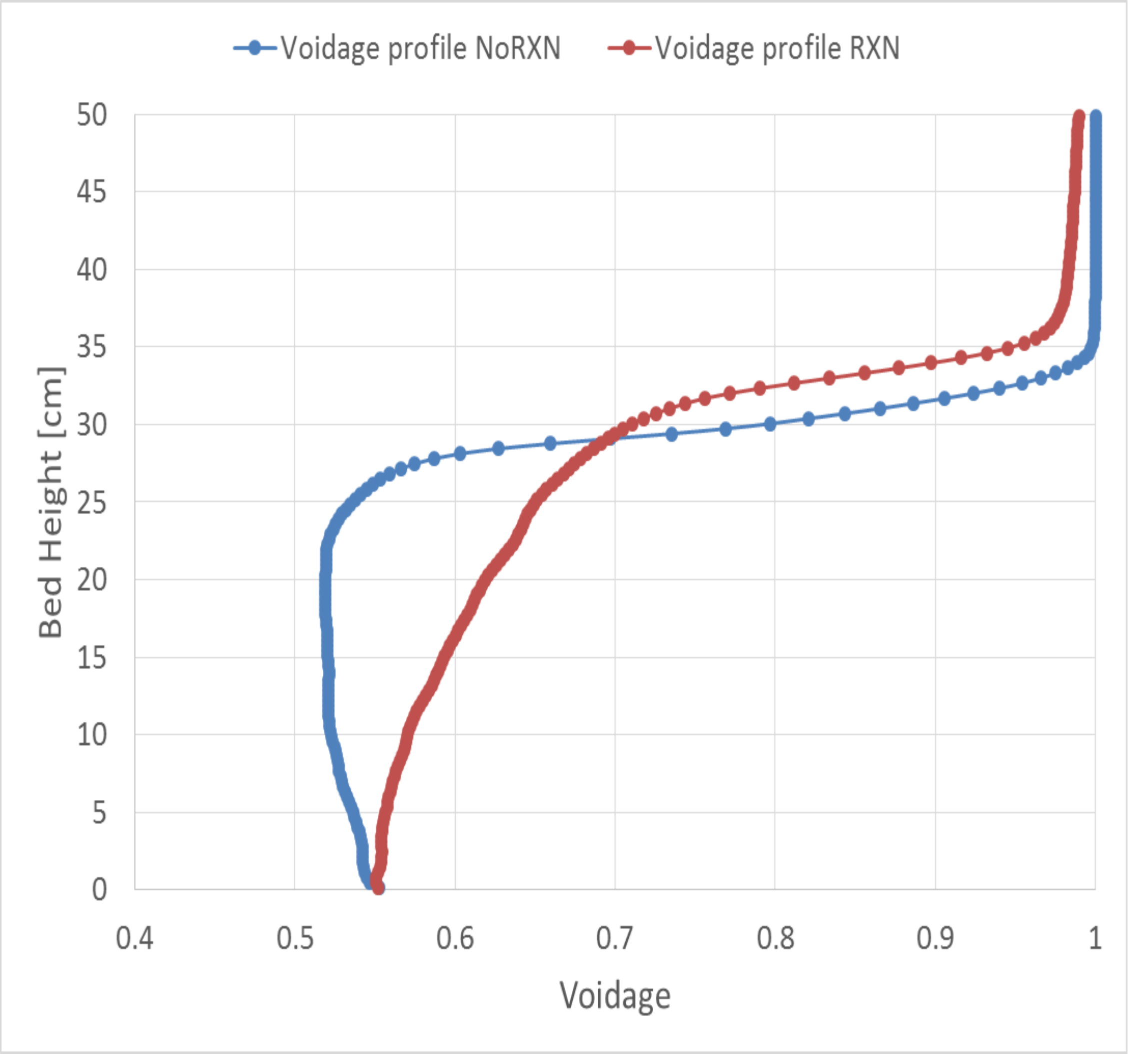
Reacting vs non-reacting hydrodynamics



Summary and future work

- Ongoing work towards validation of a reacting CFD methodology for biomass gasification in a steam environment
- Use of tools employing detailed chemistry to extract information about the global chemical mechanisms implemented in CFD
- Revisit the devolatilization mechanism by implementing more detailed schemes
- Potential effect of the emulsion phase on the water gas shift reaction
- Enhancement of reactor network models employing detailed chemistry by feeding back information about gas-solids mixing obtained from CFD

References

[1] C. Di Blassi, “Modeling chemical and physical processes of wood and biomass pyrolysis”, *Progress in Energy and Combustion Science*, **2008**, 34(1):47-90

[2] M. Syamlal, W. Rogers, T.J. O'Brien, “Mfix documentation theory guide”, *Technical Report, U.S. Department of Energy, National Energy Technology Laboratory*, **1993**

[3] M. Syamlal, W. Rogers, T.J. O'Brien, “Mfix documentation numerical technique”, *Technical Report, U.S. Department of Energy, National Energy Technology Laboratory*, **1998**

[4] D. Gera, M. Syamlal, T. O’Brien, “Hydrodynamics of particle segregation in fluidized beds”, *International Journal of Multiphase Flow*, **2004**, 30:419-428

[5] C. Altantzis, R.B. Bates, A.F. Ghoniem, “3D Eulerian modeling of thin rectangular gas–solid fluidized beds: estimation of the specularity coefficient and its effects on bubbling dynamics and circulation times”, *Powder Technology*, **2015**, 270(A):256-270

[6] A. Bakshi, C. Altantzis, R.B. Bates, A.F. Ghoniem, “Eulerian–Eulerian simulation of dense solid–gas cylindrical fluidized beds: Impact of wall boundary condition and drag model on fluidization”, *Powder Technology*, **2015**, 277:47-62

[7] M.G. Grønli, M.C. Melaaen, “Mathematical model for wood pyrolysis-comparison of experimental measurements with model predictions”, *Energy Fuels*, **2000**, 14:791–800

[8] V. Biba, J. Macak, E. Klose, J. Malecha, “Mathematical model for the gasification of coal under pressure”, *Industrial & Engineering Chemical Process Design and Development*, **1978**, 17:92

[9] M.L. Hobbs, P.T. Radulovic, L.D. Smoot, “Modeling fixed-bed coal gasifiers”, *AIChE Journal,* **1992**, 38(5):681–702

[10] Addison Stark, “Multi-Scale Chemistry Modeling of the Thermochemical Conversion of Biomass in a Fluidized Bed Gasifier”, Massachusetts Institute of Technology, PhD Thesis, **2015**